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**NONLINEAR ADJUSTMENT WITH OR WITHOUT CONSTRAINTS,
APPLICABLE TO GEODETIC MODELS**

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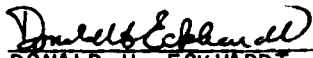


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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) <p>The present study concentrates on the least-squares resolution of the parametric adjustment model. In general, this model may occur in a linear or a nonlinear form, and may or may not have constraints associated with it. The constraints, if present, may be linear or nonlinear. Furthermore, two basic categories of constraints are available, namely the familiar equality constraints, i.e., exact relations which must be fulfilled by the parameters, and the relatively new category of inequality constraints. With the exception of the inequality constraints, which are treated in the linear version in conjunction with the linear</p>														

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parametric model, the adjustment model and the eventual (equality) constraints are presented here in the nonlinear version. But in every case, the least-squares solution is achieved via an isomorphic geometrical setup with tensor structure and notation. This is possible due to the fact that in the geometrical context the least-squares criterion translates into the minimum distance property, which, in turn, entails an orthogonal projection of the observational point onto the pertinent model surface. *May 1977*

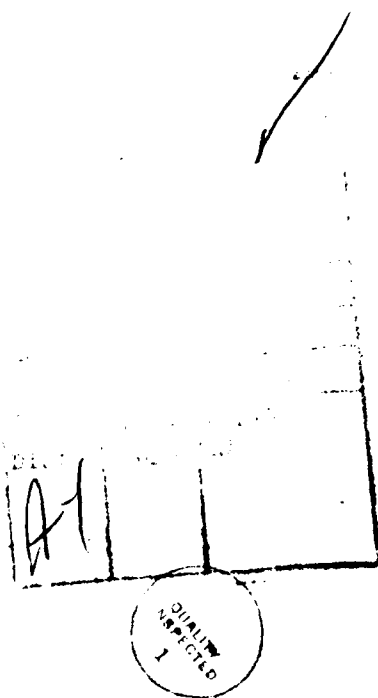


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1. INTRODUCTION

The aim of this report is to present new elements in a rigorous least-squares adjustment of geodetic quantities. Although the initial emphasis was on the satellite-to-satellite tracking (SST), the adjustment aspects developed during the course of the study are broad enough to be applicable to a variety of problems in physical sciences. The body of the report is thus reserved for the nonlinear least-squares method with or without constraints, whereas the SST model and its adjustment are described in Appendix A. The constraints are considered to be in general nonlinear; linear constraints joined to a linear model are presented merely as a special case. A relatively new category of constraints, termed inequality constraints, is treated in Appendix B.

The SST model, when considered without any approximations or deformations, such as the smoothing and differentiation of the original observations, appears to have the form of the general adjustment model. The latter usually features the observables and the parameters interwoven in nonlinear relationships. However, the observables in the SST model have special characteristics allowing for a substantial simplification. In particular, they are present in linear combinations involving merely two observables per equation. A simple linear transformation of the observables, which affects the original observations, the adjusted observations, and the residuals in the same fashion, changes the general model into the parametric adjustment model. The latter is treated here in a nonlinear form. One can thus avoid the approximations caused by the truncation of second- and higher-order terms in the model's Taylor-series expansion, as is done in the standard linearized approach. The transformation of observables leading to the parametric model can be useful not only in view of the rigorous least-squares adjustment of the SST, but in the treatment of other kinds of geodetic data as well.

The above transformation has allowed the analysis to shift focus from the general adjustment model, linear or nonlinear, to the nonlinear parametric adjustment model. The linear version of the latter follows as a simple special case; it has been thoroughly analyzed and extensively used over the past several decades. The least-squares adjustment of the nonlinear parametric model is the subject of Chapter 2, summarizing the recent development contained in the AFGL report [Blaha, 1989]. This development is based on analogies between

adjustments and geometry which have led to the conception of an isomorphic geometrical setup.

In some adjustment problems the parametric model is subject to constraints, i.e., conditions to be fulfilled by its parameters. As an illustration related to the SST, one notices that although equation (2) in Appendix A does not contain any constraints among the parameters, certain types of constraints may be needed in conjunction with the geopotential representation used by the model, and with other factors. In an early treatment of the SST, Schwarz [1970] considers the gravity field split into the reference field described by an (N,N) spherical-harmonic expansion, and the residual field described by density-layer parameters. Because of the initial stipulation that the density layer solution should not affect any of the $(N+1)^2$ coefficients in the underlying spherical-harmonic model, he concludes that $(N+1)^2$ constraints should be included, at least in theory. Clearly, this notion is not tied only to the density-layer parameters since similar reasoning applies also with regard to other localized representations of the residual gravity field.

In analogy to an adjustment model itself, a set of constraints can also be linear or nonlinear. A constrained least-squares adjustment, where the emphasis is on nonlinear constraints, is developed in Chapter 3 herein. This endeavor is again based on the isomorphism between adjustments and geometry. The geometric derivations leading to the final adjustment formulas are carried out with the aid of tensor structure and notation. It should be mentioned that all the constraints considered so far, whether linear or nonlinear, are the familiar equality constraints.

However, recent years have witnessed an increasing interest in applications of linear inequality constraints, which can be used with advantage in the problems where the smoothing effect of the standard least-squares method is undesirable. The concept of inequality constraints is instrumental in reducing the solution space to a band, as is described by Fritsch [1987] in conjunction with a linear parametric adjustment model. This, in turn, allows one to minimize the maximum error and thus to accommodate the worst case. Appendix B herein presents the least-squares algorithm applicable to linear models with linear inequality constraints, which is developed using again an isomorphic geometrical setup with tensor structure and notation.

2. NONLINEAR PARAMETRIC LEAST-SQUARES ADJUSTMENT

2.1 Mathematical Background

The parametric adjustment model expresses each of the observables in terms of parameters, where the structure linking the two groups of variables is, in general, nonlinear. The number of observables is denoted by n and the number of parameters by u , where n must be greater than u for an adjustment to take place. The adjustment model is written as

$$L^a = F(X^a) ,$$

where L^a and X^a are the sets (column-vectors) of adjusted observations and adjusted parameters, respectively. This chapter describes the resolution of a nonlinear model through an isomorphic geometrical setup with tensor structure and notation. Such efforts date back to [Blaha, 1984], which treats a linear or linearized adjustment model. Later papers and reports, such as [Blaha, 1987], contain an initial analysis of a nonlinear model. The most recent development in this area is described in [Blaha, 1989].

In a standard adjustment approach, a nonlinear adjustment model is subject to the Taylor series expansion based on an initial set of parametric values, X^0 . The terms in the second and higher powers of the parametric corrections are neglected, resulting in the familiar (linearized) observation equations. In matrix notation, the latter are expressed by

$$V = A X + L ,$$

where A is the design matrix, $X = X^a - X^0$ is the column-vector of parametric corrections, $V = L^a - L^b$ is the column-vector of residuals, and $L = L^0 - L^b$ is the column-vector of constant terms, with $L^0 = F(X^0)$ representing observables consistent with the initial set of parameters, and L^b containing the actual observations. The linearized model is subjected to the least-squares criterion

$$V^T P V = \text{minimum} ,$$

where P is the weight matrix of observations. This criterion leads to the formation of the familiar normal equations.

If the original adjustment model is nonlinear, the resolution of the linearized model does not yield the final answers. The process is usually repeated with new, updated parameters and the corresponding changes in A and L. However, the variance-covariance matrix of observations, Σ , as well as the weight matrix P, adopted as $P = \Sigma^{-1}$, are constant. Thus, the matrix of normal equations, $N = A^T P A$, changes only due to A, and the column-vector representing the right-hand side of normal equations, $U = -A^T P L$, changes only due to A and L. The computation of the updated parametric values through a new X requires the formation and the inversion of a new N in each iteration, or a mathematically equivalent procedure. When X becomes sufficiently close to zero the iterative process is terminated. As its by-product, the latest matrix N^{-1} is adopted as the variance-covariance matrix of adjusted parameters.

The functional relationship between the observables and the parameters lends itself to a geometrical interpretation and treatment involving spaces and surfaces generalized to higher dimensions. In particular, the formulation

$$x^r = x^r(u^\alpha), \quad r = 1, 2, \dots, n, \quad \alpha = 1, 2, \dots, u,$$

representing the parametric adjustment model, can be linked to the Gauss form of a surface in relation to the surrounding space, where x^r are the space coordinates and u^α are the surface coordinates. The Gauss form of a two-dimensional surface ($u=2$) embedded in a three-dimensional flat space ($n=3$) is described, together with two other forms, in Chapter 6 of [Hotine, 1969]. In [Blaha, 1984], both the n -dimensional "observational" space and the u -dimensional "model" surface were considered flat. The latter was thus in reality a hyperplane. Although the model surface is now intrinsically a curved space, the surrounding space is again flat, and, as is shown below, its coordinate system is characterized by a constant metric tensor.

In denoting the n observables by x^r , $r=1, 2, \dots, n$, and the u unknown parameters by u^α , $\alpha=1, 2, \dots, u$, we can represent a nonlinear parametric adjustment model by

$$\begin{aligned} x^r = x^r(u^\alpha) = x^r_0 + A^r_\alpha \Delta u^\alpha + (1/2) \Omega^r_{\alpha\beta} \Delta u^\alpha \Delta u^\beta \\ + (1/6) \Phi^r_{\alpha\beta\gamma} \Delta u^\alpha \Delta u^\beta \Delta u^\gamma + \dots, \end{aligned} \quad (1a)$$

$$\Delta u^\alpha = u^\alpha - u^\alpha_0, \quad (1b)$$

where u_0^α represents an initial set of parameters and $x_0^r = x^r(u_0^\alpha)$ represents the observables consistent with this set. The lower-case Roman indices range from 1 to n, and the lower-case Greek indices range from 1 to u. Tensor symbolism implies the summation convention over the dummy (repeating) indices.

In the geometrical context, the first equality in (1a) represents the Gauss form of a u-dimensional surface embedded in an n-dimensional space. The surface is endowed with the coordinate system $\{u^\alpha\}$, $\alpha=1,2,\dots,u$ and is referred to as the model surface, and the space is endowed with the coordinate system $\{x^r\}$, $r=1,2,\dots,n$, and is referred to as the observational space. The second equality in (1a) is the Taylor series expansion of x^r from the "initial" point P lying in the model surface, whose model-surface coordinates are u_0^α and whose observational-space coordinates are x_0^r . The notation identifying the partial derivatives at P, such as $\partial x^r / \partial u^\alpha = A_\alpha^r$, $\partial^2 x^r / \partial u^\alpha \partial u^\beta = \Omega_{\alpha\beta}^r$, etc., is self-evident. The actual observations can be thought of as describing the point Q in the observational space, which, due to measuring errors, does not lie in the known model surface. The task at hand consists in determining, from the observed point Q, a model-surface point satisfying the least-squares criterion.

In the adjustment context, the variance-covariance and the weight matrices of observations depend on the quality of measurements. They are independent of the adjustment model, of the initial set of parameters, of the outcome of observations, etc. Thus, for a given observational mode they are constant. In the "traditional" identification of [Blaha, 1984], variance-covariance matrices correspond to associated metric tensors, and weight matrices correspond to metric tensors. Accordingly, we represent the variance-covariance matrix of observations by the observational-space associated metric tensor g^{rs} , and the weight matrix of observations by the observational-space metric tensor g_{sr} , and state that both tensors are independent of the form of the model surface, of the initial point P, of the observed point Q, etc., leading to the simplification

$$g_{sr} = \text{constant} \quad (2)$$

One could also attribute the tensors g^{rs} and g_{sr} to the point Q and state that the geometrical setup must account for Q located anywhere in the observational space. In turn, (2) implies that the observational space must be flat.

If the set $\delta \bar{x}^r$ denotes the coordinate differences between the observed point Q and the desired model-surface point denoted \bar{P} , it corresponds to the negative residuals, and the least-squares criterion corresponds to

$$\delta \bar{s}^2 = \delta \bar{x}^s g_{sr} \delta \bar{x}^r = \text{minimum} . \quad (3)$$

The quadratic form (3) represents the square of the distance between Q and \bar{P} . Therefore, the desired "least-squares" point \bar{P} must be the foot-point of the straight line dropped orthogonally from Q onto the model surface. We note that if any other adjustment condition were used in lieu of the least-squares criterion, the minimum distance property (3) would not exist and the geometric-tensorial treatment of the adjustment theory would probably be much more complex if not impossible.

2.2 Summary of the Geometrical Development

A convenient approach for resolving nonlinear least-squares problems consists in using an isomorphic geometrical setup with tensor structure and notation. Such a link is highlighted by the consideration that the least squares criterion gives rise to a minimum distance property. Among the basic correspondences, the number of observations, n , and the number of parameters, u , define the dimensionality of the observational space and of the model surface, respectively. Since the constant variance covariance matrix of observations, Σ , corresponds to the associated metric tensor g^{rs} , and the weight matrix of observations, adopted as Σ^{-1} , corresponds to the metric tensor g_{sr} , the observational space is endowed with a coordinate system $\{x^r\}$ such that

$$g_{sr} = \text{constant} , \quad g^{rs} = \text{constant} .$$

The set L^b of actual observations corresponds to the set x_Q^r of observational-space coordinates describing the point Q. All possible sets of adjusted observations (subject to no criterion) correspond to the Gauss form of the model surface endowed with a coordinate system $\{u^\alpha\}$:

$$x^r = x^r(u^\alpha) , \quad r = 1, 2, \dots, n , \quad \alpha = 1, 2, \dots, u .$$

The final set of adjusted parameters, x^a , corresponds to a particular set u^α of model-surface coordinates describing the least squares point \bar{P} . The set

of initial parameters, X^0 , corresponds to the set u_0^α of model-surface coordinates describing the initial point P. The final set of parametric corrections, X , then corresponds to $\Delta u^\alpha = u^\alpha - u_0^\alpha$; these quantities are assumed to be small (termed first-order). The final set of adjusted observations, $L^a = F(X^a)$, corresponds to a particular set $x^r = x^r(u^\alpha)$ of observational-space coordinates describing the least-squares point \bar{P} . The initial point P is described by these coordinates as $x_0^r = x^r(u_0^\alpha)$, reflecting its counterpart $L^0 = F(X^0)$. The set of negative constant terms, $-L = L^b - F(X^0)$, corresponds to the contravariant vector $\delta x^r = x_Q^r - x_0^r$, while the set of negative residuals, $-V = L^b - L^a$, corresponds to the contravariant vector $\delta x^r = x_Q^r - x^r$. The initial design matrix, A , which in standard observation equations, $V = AX + L$, relates the parametric corrections to the residuals, corresponds to the design tensor $A_\alpha^r = \partial x^r / \partial u^\alpha$ evaluated at P. On the other hand, the standard adjustment approach does not have equivalents of $\Omega_{\alpha\beta}^r$ and $\Phi_{\alpha\beta\gamma}^r$, which form three- and four dimensional arrays, respectively, and contain the second- and the third-order partial derivatives of x^r with respect to u^α , evaluated at P.

The geometrical approach is based on a direct exploitation of the relation

$$\bar{A}_\beta^s g_{sr} \delta x^r = 0, \quad (4)$$

where \bar{A}_β^s represents the design tensor evaluated at the least-squares point \bar{P} , and equation (4) itself represents the orthogonality condition at \bar{P} . The outcome of the geometrical development is considered in two methods, called geometrical and extended geometrical. It is contrasted to the standard method treating nonlinear models in a linearized form. The algorithms associated with all three methods are presented below in the form of the first iteration, and in the form of the second and subsequent iterations.

In tensor notation, the initial matrix of normal equations corresponds to the model-surface metric tensor $a_{\beta\alpha}$ at the initial point P, and the initial right-hand side of normal equations corresponds to the model-surface covariant vector $A_\beta^s \delta x_s$ at P, where

$$a_{\beta\alpha} = A_\beta^s g_{sr} A_\alpha^r, \quad \delta x_s = g_{sr} \delta x^r.$$

The parametric corrections stemming from the first iteration are symbolized by (Δu^α) , and they give rise to an updated point (P). The latter is described by the model-surface coordinates $(u^\alpha) = u_0^\alpha + (\Delta u^\alpha)$. The quantities belonging to (P)

will likewise be written in parentheses. The parametric corrections obtained in the second iteration will be denoted $\Delta(\Delta u^\alpha)$, and they will give rise to a new updated point determined via $(u^\alpha) + \Delta(\Delta u^\alpha)$. The notation used in conjunction with the second iteration will be retained also for any further iterations.

Standard method. Under the assumption that both sets Δu^α and δx^r contain small quantities (first-order), the first iteration in the standard method reads

$$a_{\beta\alpha} (\Delta u^\alpha) = A_\beta^s \delta x_s, \quad (5a)$$

representing the initial normal equations. The second and further iterations follow the same principle:

$$(a_{\beta\alpha}) \Delta(\Delta u^\alpha) = (A_\beta^s) (\delta x_s). \quad (5b)$$

Geometrical method. Under the same assumption as above (both sets Δu^α and δx^r contain small quantities), the first iteration utilizes the same formula as its standard counterpart, namely

$$a_{\beta\alpha} (\Delta u^\alpha) = A_\beta^s \delta x_s. \quad (6a)$$

However, the second and further iterations proceed according to

$$[(a_{\beta\alpha}) - (\delta x_s) \Omega_{\beta\alpha}^s] \Delta(\Delta u^\alpha) = (A_\beta^s) (\delta x_s), \quad (6b)$$

representing the modified normal equations. The triply-indexed quantity $\Omega_{\beta\alpha}^s$, formed by second-order partial derivatives of the observables with respect to the parameters, is evaluated only at the initial point P.

Extended geometrical method. Although the assumption regarding Δu^α is unchanged, this method is tailored for δx^r containing relatively large quantities, for which the first iteration reads

$$[a_{\beta\alpha} - \delta x_s \Omega_{\beta\alpha}^s] (\Delta u^\alpha) = A_\beta^s \delta x_s. \quad (7a)$$

Compared to the geometrical method, the current algorithm is seen to utilize second-order partial derivatives and to give rise to the modified normal equations already in its first iteration. The formula for the second and further iterations is given as

$$[(a_{\beta\alpha}) - (\delta x_s) \Omega_{\beta\alpha}^s - (\delta x_s) \Phi_{\beta\alpha\gamma}^s (\Delta u^\gamma)] \Delta(\Delta u^\alpha) = (A_\beta^s) (\delta x_s), \quad (7b)$$

representing the modified normal equations at updated stages. Here use is made of $\phi_{\beta\alpha\gamma}^s$ containing third-order partial derivatives. This quantity is evaluated only at P, similar in this respect to $\Omega_{\beta\alpha}^s$. We note that the quantity inside the brackets of (7b) could be replaced by $(a_{\beta\alpha}) - (\delta x_s)(\Omega_{\beta\alpha}^s)$, where $(\Omega_{\beta\alpha}^s)$ would represent the second-order partial derivatives evaluated at an updated point.

The standard adjustment algorithm, represented by the relations (5a,b) above, results in the projection of the point Q onto the model plane passing through the initial point P, followed by the projection of Q onto a new model plane passing through an updated point (P), etc. The orthogonality condition (4) is then fulfilled essentially as a by-product of these projections. By contrast, the geometrical approach actively seeks to fulfill it at every step. A one-step solution producing the least-squares point \bar{P} directly is hindered only by the necessity to truncate certain terms, but not to the extent of making the entire model linear (see the above equations 6b and 7a,b). The matrix of modified normal equations generated in the process is positive-definite, similar in this respect to the matrix of normal equations in the standard method.

Encouraging results have been obtained in the numerical example presented in the Appendix of [Blaha, 1989], illustrating convergence properties of an adjustment of a third-order polynomial in four variables. Although the standard method converged slowly in one of four analyzed cases and diverged in two others, the geometrical method converged in two and three iterations, respectively. The extended geometrical method further reduced the number of iterations from three to two. It is expected that in most nonlinear cases the presence of second-order partial derivatives will translate into two iterations in the geometrical method as compared to several iterations needed by the standard method.

3. ADJUSTMENT WITH NONLINEAR CONSTRAINTS

3.1 Initial Relations in Matrix Notation

This chapter is concerned with the introduction of nonlinear constraints into a nonlinear least-squares adjustment model. In standard adjustment notation, a set of s constraints among u parameters is symbolized by

$$G(X^a) = 0 ,$$

where X^a represents the set (column-vector) of adjusted parameters. The usual approach consists in expanding these constraints in the Taylor series using an initial set of parametric values, symbolized by X^0 . It then follows that

$$G(X^a) = W_c + C X + \dots = 0 ,$$

where

$$W_c = G(X^0) , \quad C = (\partial G / \partial X)_0 ,$$

and where $X = X^a - X^0$ is a set of parametric corrections. The subscript "o" indicates that the matrix C is evaluated using the elements of X^0 . This matrix has the dimensions $s \times u$, while the column vectors W_c and X contain s and u elements, respectively. In a standard (linearized) approach, the terms symbolized above by dots are omitted.

Here, as well as in standard adjustment theory, the constraints are considered independent, in the sense that the constraint matrix C has the full row rank s . However, the standard theory proceeds in general with $W_c \neq 0$. By contrast, the current nonlinear development will benefit from such initial values X^0 for which it holds true that

$$G(X^0) = 0 . \tag{8}$$

In this case, only $u-s$ of the u values in X^0 can be chosen independently. Although a set X^0 for which $G(X^0) \neq 0$ would also be acceptable, the computations which below will lead to $G(X^0) = 0$ would eventually have to be performed as well, and the resulting formulas would be more cumbersome and less tractable.

A simple iterative algorithm leading to $G(X^0) = 0$ can be presented as follows. First, the matrix C is partitioned into $[C_1 \ C_2]$, where the submatrices C_1 and C_2 have the dimensions $s \times (u-s)$ and $s \times s$, respectively. The submatrix C_2

can be considered nonsingular without any loss of generality, since, if needed, the parameters could always be rearranged beforehand for this condition to be satisfied. The vector X^0 is similarly partitioned into the subsets denoted temporarily X_1 and X_2 , which contain u-s and s elements, respectively. The elements of X_1 are chosen independently, and are thus held fixed throughout. The remaining elements, grouped in X_2 , are subject to change. We symbolize their initial choice by X_2^0 to accommodate the iterative indices below. The first iteration yields corrections grouped in ΔX_2^1 , resulting in an improved vector denoted X_2^1 . After an i-th iteration, this vector becomes

$$X_2^i = X_2^{i-1} + \Delta X_2^i .$$

If the corrections become negligible and the iterative process is terminated after n iterations, the values in X_2^n are adopted as the elements of X_2 . In joining this vector to the independently chosen vector X_1 , one obtains the desired vector X^0 .

The model before the i-th iteration can be presented as follows:

$$G(X^0) \equiv G(X_1, X_2) = G(X_1, X_2^{i-1}) + C_2^{i-1} (X_2 - X_2^{i-1}) + \dots = 0 ,$$

resulting in the i-th solution:

$$X_2 - X_2^{i-1} = -(C_2^{i-1})^{-1} G(X_1, X_2^{i-1}) + \dots .$$

Upon neglecting the higher-order terms represented by the dots, one obtains

$$\Delta X_2^i \equiv X_2^i - X_2^{i-1} = -(C_2^{i-1})^{-1} G(X_1, X_2^{i-1}) .$$

If the values in ΔX_2^i are not deemed negligible, the matrix C_2 is updated upon evaluating $\partial G / \partial X_2$ with the new values X_2^i , and is denoted C_2^i . Similarly, one forms an updated vector $G(X_1, X_2^i)$ and proceeds to the iteration i+1. After the final X^0 has been computed by this or a similar procedure, an actual nonlinear least-squares adjustment with constraints can take place.

3.2 Parametric Elimination Due to Constraints

As we have seen in (1a,b) of Chapter 2, the nonlinear parametric adjustment model can be written as

$$x^r(u^\alpha) = x^r(u_0^\alpha) + A_\alpha^r \Delta u^\alpha + (1/2) \Omega_{\alpha\beta}^r \Delta u^\alpha \Delta u^\beta + \dots, \quad (9a)$$

where

$$\Delta u^\alpha = u^\alpha - u_0^\alpha, \quad (9b)$$

with $r=1,2,\dots,n$, $\alpha=1,2,\dots,u$; and where

$$A_\alpha^r = (\partial x^r / \partial u^\alpha)_0, \quad \Omega_{\alpha\beta}^r = (\partial^2 x^r / \partial u^\alpha \partial u^\beta)_0, \dots$$

All lower-case Greek letters vary in the fashion prescribed above for α . A similar convention applies for other kinds of indices as well (lower-case Roman letters, etc.). The subscript "0" indicates the evaluation at the initial point P lying in the model surface.

The s nonlinear constraints joined to this model are represented by

$$G^L(u^\alpha) = 0, \quad (10a)$$

where $L=1,2,\dots,s$. This equation can be regarded as the functional form of a surface, generalized to higher dimensions. In referring to (8) in the preceding section, one also has

$$G^L(u_0^\alpha) = 0, \quad (10b)$$

where the values u_0^α , $\alpha=1,2,\dots,u$, are known. The functional form (10a) restricts the final least-squares point, whose model-surface coordinates are u^α , to a certain lower-dimensional surface embedded in the model surface. From (10b) it follows that the initial point P also belongs to this lower-dimensional surface, which will be called "model subsurface". This is apparent from the right-hand sides of (10a,b), which contain the same sets of constants (zeros).

The current development is organized along the following lines. First, the coordinate set $\{u^\alpha\}$, $\alpha=1,2,\dots,u$, is partitioned into $\{u^\Lambda, u^K\}$, $\Lambda=1,2,\dots,u-s$, $K=1,2,\dots,s$. This allows (10a) to be written as

$$G^L(u^\Lambda, u^K) = 0, \quad (11)$$

representing the functional form of the model subsurface. Subject to the condition stated explicitly in the sequel, (11) makes it possible to express the last s coordinates in terms of the first u s coordinates:

$$u^K = u^K(u^\Lambda) \quad (12)$$

Equation (12) is the Monge form of the model subsurface embedded in the model surface, where u^Λ , $\Lambda=1,2,\dots,u$ -s, are the subsurface coordinates (independent variables). The substitution of (12) into (11) yields

$$g^L(u^\Lambda) \equiv G^L(u^\Lambda, u^K(u^\Lambda)) = 0 \quad (13)$$

which is an identity in the model subsurface. Thus, further identities follow:

$$\partial g^L / \partial u^\Lambda = 0 \quad , \quad \partial^2 g^L / \partial u^\Lambda \partial u^\Omega = 0 \quad , \quad \dots \quad (14a,b)$$

leading to a relation for $u^K(u^\Lambda)$. In this way, the parameters u^K , $K=1,2,\dots,s$, will have been effectively eliminated.

Expressed in the Taylor series, (10a) reads

$$g^L(u^\alpha) \equiv C_\alpha^L \Delta u^\alpha + (1/2) H_{\alpha\beta}^L \Delta u^\alpha \Delta u^\beta + \dots = 0 \quad ,$$

where advantage has been taken of (10b), and where

$$C_\alpha^L = (\partial g^L / \partial u^\alpha)_0 \quad , \quad H_{\alpha\beta}^L = (\partial^2 g^L / \partial u^\alpha \partial u^\beta)_0 \quad , \quad \dots$$

In using the partition of $\{u^\alpha\}$ and the symmetry of partial derivatives in the lower-case Greek indices, one develops this equation as

$$\begin{aligned} g^L(u^\Lambda, u^K) \equiv & C_\Lambda^L \Delta u^\Lambda + C_K^L \Delta u^K + (1/2) [H_{\Lambda\Omega}^L \Delta u^\Lambda \Delta u^\Omega \\ & + 2 H_{\Lambda K}^L \Delta u^\Lambda \Delta u^K + H_{KM}^L \Delta u^K \Delta u^M] + \dots = 0 \quad , \end{aligned} \quad (15a)$$

where

$$\Delta u^\Lambda = u^\Lambda - u_0^\Lambda \quad , \quad \Delta u^K = u^K - u_0^K \quad , \quad (15b,c)$$

and where u_0^Λ , u_0^K , the model-surface coordinates of P , are known (see the relation 10b and the statement below it). Equation (15a) corresponds to the step represented by (11). In evoking (12), we next formulate the Taylor series for u^K :

$$\Delta u^K = A_\Lambda^K \Delta u^\Lambda + (1/2) \Omega_{\Lambda\Omega}^K \Delta u^\Lambda \Delta u^\Omega + \dots \quad (16)$$

where

$$A'^K_{\Lambda} = (\partial u^K / \partial u^{\Lambda})_0, \quad \Omega'^K_{\Lambda\Omega} = (\partial^2 u^K / \partial u^{\Lambda} \partial u^{\Omega})_0, \dots$$

The partial derivatives are again symmetric in the pertinent indices.

The substitution of (16) into (15a) in view of the step (13) yields

$$\begin{aligned} g^L(u^{\Lambda}) &\equiv C^L_{\Lambda} \Delta u^{\Lambda} + C^L_K A'^K_{\Lambda} \Delta u^{\Lambda} + (1/2) C^L_K \Omega'^K_{\Lambda\Omega} \Delta u^{\Lambda} \Delta u^{\Omega} \\ &+ (1/2) H^L_{\Lambda\Omega} \Delta u^{\Lambda} \Delta u^{\Omega} + H^L_{\Lambda K} \Delta u^{\Lambda} A'^K_{\Omega} \Delta u^{\Omega} \\ &+ (1/2) H^L_{KM} A'^K_{\Lambda} \Delta u^{\Lambda} A'^M_{\Omega} \Delta u^{\Omega} + \dots = 0. \end{aligned}$$

This identity is immediately confirmed at P. Upon differentiating it in succession in accordance with the step (14a,b), and rearranging the free as well as the dummy indices, it follows that

$$\begin{aligned} \partial g^L / \partial u^{\Lambda} &\equiv C^L_{\Lambda} + C^L_K A'^K_{\Lambda} - C^L_K \Omega'^K_{\Lambda\Omega} \Delta u^{\Omega} + H^L_{\Lambda\Omega} \Delta u^{\Omega} \\ &+ H^L_{\Lambda K} A'^K_{\Omega} \Delta u^{\Omega} + H^L_{\Omega K} \Delta u^{\Omega} A'^K_{\Lambda} \\ &+ H^L_{KM} A'^K_{\Omega} \Delta u^{\Omega} A'^M_{\Lambda} + \dots = 0, \end{aligned} \quad (17)$$

$$\begin{aligned} \partial^2 g^L / \partial u^{\Lambda} \partial u^{\Omega} &\equiv C^L_K \Omega'^K_{\Lambda\Omega} + H^L_{\Lambda\Omega} + H^L_{\Lambda K} A'^K_{\Omega} + H^L_{\Omega K} A'^K_{\Lambda} \\ &+ H^L_{KM} A'^M_{\Omega} A'^K_{\Lambda} + \dots = 0, \end{aligned} \quad (18)$$

where the dots represent terms containing Δu^{Ω} , $\Delta u^{\Omega} \Delta u^{\Psi}$, etc. There is no need to present partial derivatives of higher order than those featured in (17), (18).

The evaluation of (17) and (18) at P yields, respectively,

$$A'^K_{\Lambda} = - D^K_L C^L_{\Lambda}, \quad (19)$$

$$\Omega'^K_{\Lambda\Omega} = - D^K_L [H^L_{\Lambda\Omega} + H^L_{\Lambda M} A'^M_{\Omega} + (H^L_{\Omega M} + H^L_{MN} A'^N_{\Omega}) A'^M_{\Lambda}], \quad (20)$$

where

$$D^M_L C^L_K = \delta^M_K.$$

The last equation represents the condition mentioned below (11). In matrix notation, this condition states that the matrix $[D^M_L]$ is the inverse of $[C^L_K]$, which in turn implies that the matrix $[C^L_K]$ of dimensions $s \times u$ must have the full row rank s , and, therefore, that the constraints must be linearly

independent. In the affirmative, an eventual rearranging of parameters will ensure that the matrix $[C_K^L]$ is regular (i.e., square and nonsingular). This subject has already been discussed in Section 3.1, and has led to (10b). Upon substituting (19), (20), and higher order partial derivatives (not listed) into (16), one obtains a relationship for u^K as has been indicated below (14a,b).

Next, Δu^K from (16) is substituted into (9a). Upon the realization that

$$A_{\alpha}^r \Delta u^{\alpha} = A_{\Lambda}^r \Delta u^{\Lambda} + A_K^r \Delta u^K,$$

$$\Omega_{\alpha\beta}^r \Delta u^{\alpha} \Delta u^{\beta} = \Omega_{\Lambda\Omega}^r \Delta u^{\Lambda} \Delta u^{\Omega} + 2 \Omega_{\Lambda K}^r \Delta u^{\Lambda} \Delta u^K + \Omega_{KM}^r \Delta u^K \Delta u^M,$$

this substitution yields

$$\begin{aligned} x^r - x_0^r &= (A_{\Lambda}^r + A_K^r A_{\Lambda}^{\prime K}) \Delta u^{\Lambda} + (1/2) (\Omega_{\Lambda\Omega}^r + A_K^r \Omega_{\Lambda\Omega}^{\prime K} \\ &+ 2 \Omega_{\Lambda K}^r A_{\Omega}^{\prime K} + \Omega_{KM}^r A_{\Lambda}^{\prime K} A_{\Omega}^{\prime M}) \Delta u^{\Lambda} \Delta u^{\Omega} + \dots, \end{aligned} \quad (21)$$

where $A_{\Lambda}^{\prime K}$, $\Omega_{\Lambda\Omega}^{\prime K}$, ..., are known from (19), (20), The symbols x^r and x_0^r in (21) are interpreted as

$$x^r = x^r(u^{\alpha}) = x^r(u^{\Lambda}, u^K(u^{\Lambda})) = \tilde{x}^r(u^{\Lambda}),$$

$$x_0^r = x^r(u_0^{\alpha}) = x^r(u_0^{\Lambda}, u^K(u_0^{\Lambda})) = \tilde{x}^r(u_0^{\Lambda}),$$

where x_0^r is known.

Equation (21) is now reformulated to read

$$\tilde{x}^r(u^{\Lambda}) = \tilde{x}^r(u_0^{\Lambda}) + \tilde{A}_{\Lambda}^r \Delta u^{\Lambda} + (1/2) \tilde{\Omega}_{\Lambda\Omega}^r \Delta u^{\Lambda} \Delta u^{\Omega} + \dots, \quad (22)$$

where the sets of implicit partial derivatives at P, namely

$$\tilde{A}_{\Lambda}^r = (\partial \tilde{x}^r / \partial u^{\Lambda})_0, \quad \tilde{\Omega}_{\Lambda\Omega}^r = (\partial^2 \tilde{x}^r / \partial u^{\Lambda} \partial u^{\Omega})_0, \dots$$

follow readily from (21):

$$\tilde{A}_{\Lambda}^r = A_{\Lambda}^r + A_K^r A_{\Lambda}^{\prime K} \quad (23a)$$

$$\tilde{\Omega}_{\Lambda\Omega}^r = \Omega_{\Lambda\Omega}^r + A_K^r \Omega_{\Lambda\Omega}^{\prime K} + 2 \Omega_{\Lambda K}^r A_{\Omega}^{\prime K} + \Omega_{KM}^r A_{\Lambda}^{\prime K} A_{\Omega}^{\prime M} \quad (23b)$$

Whereas equation (9a) represents a nonlinear model in the parameters u^{α} , $\alpha=1,2,\dots,u$, equation (22) represents a nonlinear model in the parameters u^{Λ} .

$\alpha = 1, 2, \dots, n-s$. In geometrical terms, u^α are the model surface coordinates of the point depicting the unconstrained least squares solution, and u^Λ are the model subsurface coordinates of the point depicting the constrained least-squares solution. The constrained solution can be carried out using the geometrical algorithms described in Section 2.2 (see the geometrical method or the extended geometrical method). However, having eliminated the s parameters u^K , one now has a smaller system to resolve.

3.3 Linear Constraints as a Special Case

In this section, we consider linear constraints in conjunction with the parametric adjustment model, which can be either linear, or nonlinear as in Chapter 2. Linear constraints (10a) would imply

$$H_{\alpha\beta}^L = 0, \dots$$

from which it would follow that

$$\Omega_{\Lambda\Omega}^K = 0, \dots \quad (24)$$

This outcome would lead to a simplification in the formula (23b), where the second term in the expression giving $\tilde{\Omega}_{\Lambda\Omega}^r$ would be zero.

Should the parametric model itself be linear, we would further have

$$\Omega_{\alpha\beta}^r = 0, \dots$$

This, in conjunction with (24), would yield

$$\tilde{\Omega}_{\Lambda\Omega}^r = 0, \dots \quad (25)$$

In such a case, (22) would become

$$\tilde{x}^r(u^\Lambda) = \tilde{x}^r(u_0^\Lambda) + \tilde{A}_\Lambda^r \Delta u^\Lambda, \quad (26a)$$

where

$$\tilde{A}_\Lambda^r = A_\Lambda^r + A_K^r A_\Lambda^K \quad (26b)$$

Equations (26a,b) represent a linear parametric adjustment model, where the original design tensor A_α^r is replaced by \tilde{A}_Λ^r , and the original set Δu^α is replaced by Δu^Λ . As in the preceding section, this system is smaller than the original one, due to the elimination of the parameters u^K .

The above elimination can be confirmed in the standard adjustment notation as follows. In a linear model, the exact observation equations read

$$V = A X + L, \quad (27)$$

where $L = L^0 - L^b$ and $X = X^a - X^0$, as defined earlier. The design matrix A is now constant regardless of the set X^0 . The linear constraints are expressed by

$$G(X^a) = p + C X^a = 0, \quad (28a)$$

where p is a known constant set of s elements and, in analogy to A , the matrix C is constant. In agreement with (8), we use the initial values X^0 such that

$$G(X^0) = p + C X^0 = 0, \quad (28b)$$

and state that only a u -s subset of X^0 can be chosen independently. In partitioning C as in Section 3.1, i.e., $C = [C_1 \ C_2]$, and partitioning X^0 similarly as $X^0 = [X_1^{0T} \ X_2^{0T}]^T$, where X_1^0 is the chosen subset, from (28b) we have

$$X_2^0 = -C_2^{-1} (p + C_1 X_1^0). \quad (29)$$

Due to (28a,b), we can write

$$C X = 0. \quad (30)$$

In partitioning $X = [X_1^T \ X_2^T]^T$ from (30) we deduce, similar to (29):

$$X_2 = -C_2^{-1} C_1 X_1. \quad (31)$$

If A in (27) is partitioned in accordance with X as $[A_1 \ A_2]$, it follows that

$$V = A_1 X_1 + A_2 X_2 + L.$$

However, the substitution of (31) into this relation yields

$$V = \tilde{A}_1 X_1 + L, \quad (32a)$$

where

$$\tilde{A}_1 = A_1 - A_2 C_2^{-1} C_1. \quad (32b)$$

The matrices C_2^{-1} and C_1 have already been used in forming X_2^0 in (29). We observe that the system (32a,b) corresponds to (26b) together with (19).

4. CONCLUSION

Many geodetic problems are either presented in the form of a parametric model, or can acquire this form upon a simple linear transformation of observables. A good example of this transformation is offered by the SST adjustment model. The variance covariance matrix of the original observations in such cases must be transformed accordingly, if the rigor of the adjustment is not to be compromised. The most widely accepted method of adjustment, the least-squares method, is used in practice for models that are linear, or have been linearized. By contrast, the least-squares approach presented herein focuses on the nonlinear parametric adjustment model which may, furthermore, contain a set of nonlinear constraints among the parameters.

The resolution of the nonlinear parametric adjustment model without constraints is addressed through an isomorphic geometrical setup with tensor structure and notation, represented by a u dimensional model surface embedded in a flat n -dimensional observational space. The n observations correspond to the observational-space coordinates of the point Q , the u initial parameters correspond to the model-surface coordinates of the initial point P , and the u adjusted parameters correspond to the model surface coordinates of the least-squares point \bar{P} . The least squares criterion results in a minimum distance property implying that the vector $\bar{P}Q$ must be orthogonal to the model surface. The geometrical setup leads to the solution of modified normal equations, characterized by a positive-definite matrix. The latter contains second-order and, optionally, third-order partial derivatives of the observables with respect to the parameters. This approach significantly shortens the convergence process as compared to the standard (linearized) method.

The nonlinear parametric adjustment model with nonlinear constraints is also resolved through geometrical analogies. In this situation, a point representing the least squares solution is restricted to lie in the model subsurface, i.e., a surface of smaller dimensions than the model surface in which it is embedded. The geometrical approach leads to the replacement of the model surface by the model subsurface, and to the treatment of the observational point Q with respect to the new surface in the manner that resulted in the (unrestricted) least-squares point P . Accordingly, the constrained least-squares point is the result of an orthogonal projection of Q onto the model

subsurface. In the adjustment terminology, this approach eliminates s of the original u parameters, where s is also the number of constraints. The remaining parameters are resolved by the method of the nonlinear parametric least-squares adjustment without constraints, where all the arrays must be properly modified.

A special class of constraints is represented by inequality constraints, which are treated here in a linear form, and are considered in conjunction with a linear parametric adjustment model. The isomorphic geometrical setup is now partly simplified, in the sense that general surfaces are replaced by hyperplanes. The topic of inequality constraints differs from its equality counterpart in that only some constraints (termed binding) are retained and subsequently enforced as equality constraints, whereas the remaining constraints (called nonbinding) are ignored. The most difficult question, then, is to determine which of the constraints should be retained as binding. In the geometrical context, this problem is addressed by orthogonally projecting the point representing the unrestricted least squares solution from an original model hyperplane onto appropriate hyperplanes of lower dimensions. Since orthogonal projections result in the shortest possible distance between the unrestricted least squares point and the final constrained point, the solution belongs to the least squares category.

The geometrical approach to inequality constraints is compared with the standard resolution of the same least squares problem via quadratic programming. A numerical example with four parameters is solved by both methods, leading to identical results. The main difference between the two methods is conceptual. The former attributes a clearcut geometrical meaning to every adjustment quantity, and reaches the constrained least squares solution in accordance with geometrical principles. The latter is based on algebraic principles, the key element of which is the Gauss Jordan pivoting. On the operational level, the numerical systems treated by the geometrical algorithm become progressively smaller after each orthogonal projection along a given path. By contrast, the size of such systems treated by the quadratic programming algorithm remains constant. Another advantage of the geometrical approach consists in an early detection of a path leading to a non least squares solution.

APPENDIX A

RIGOROUS ADJUSTMENT OF SATELLITE-TO-SATELLITE TRACKING DATA

In this appendix, we describe the adjustment model of the satellite-to-satellite tracking (SST), and, subsequently, a nonlinear least-squares method consistent with such a model. The observations in the SST, whether in the high-low or the low-low configurations, are the relative velocities between two satellites. These range-rate data, the error characteristics of which are assumed to be known, serve in the determination of the detailed gravity field of the earth.

SST Adjustment Model

In terms of the adjustment model, the observables are represented by intersatellite range rates and the unknown parameters are represented by selected gravity field parameters and other desired quantities. In a standard procedure, applied to a variety of problems in physical sciences, the adjustment model is linearized, whereupon range-rate observations give rise to observation equations. This system can then be resolved by the parametric method (also called the observation equation method) of the least-squares theory. It should be pointed out, however, that the intersatellite range rate does not provide a direct measure of the potential at the satellite positions. A more direct relationship would be obtained if the observables were intersatellite velocity rates, i.e., relative accelerations between two satellites.

This point is illustrated in inertial Cartesian coordinates with familiar vector notations (here the vectors are underlined). With $i=1,2$, \underline{X}_i is the position vector of the satellite i , $\dot{\underline{X}}_i$ is its velocity vector, R is the magnitude of the relative-position vector between the two satellites, \underline{e} is their unit relative-position vector, and \dot{R} is their range rate. The latter is the projection of the relative-velocity vector onto the relative-position vector:

$$\dot{R} = (\dot{\underline{X}}_2 - \dot{\underline{X}}_1) \cdot \underline{e} .$$

$$\underline{e} = (\underline{X}_2 - \underline{X}_1) / R , \quad R = |\underline{X}_2 - \underline{X}_1| .$$

The quantity central to the determination of the gravity field is the time derivative of \dot{R} , obtained by numerical differentiation. The new quantity \ddot{R} , i.e., the relative acceleration between the two satellites, can be directly related to the potential at satellite positions. The acceleration vector is numerically equal to the gradient of the gravitational potential. We thus have

$$\ddot{R} \equiv d\dot{R}/dt = a + b ,$$

where

$$a = (\nabla V_2 - \nabla V_1) \cdot \underline{e} ,$$

$$b = [(\dot{\underline{X}}_2 - \dot{\underline{X}}_1) \cdot (\dot{\underline{X}}_2 - \dot{\underline{X}}_1) - \dot{R}^2]/R .$$

Here V_i denotes the potential at the satellite position i and ∇V_i is the gradient of V_i . The main contribution of the relative acceleration between the two satellites is contained in the term a , which is the projection of the relative-acceleration vector onto the relative-position vector.

Although the relative acceleration \ddot{R} is highly suitable for modeling the gravitational potential as evidenced by the term a above, it is not an observed but a derived quantity. It is usually obtained by a curve-fitting procedure, i.e., by the filtering and the smoothing of the original observations \dot{R} , followed by a numerical differentiation with respect to time. There exist different methods, such as the spline method, for converting the original relative-velocity observations \dot{R} into the relative-acceleration "observations" \ddot{R} . Various aspects of such methods are described, for example, in [Rummel et al., 1976] and in [Hajela, 1977]. During this mathematical treatment, the original data are modified (by curve fitting), and the modified data are then transformed into quantities of a different kind (by numerical differentiation). The resulting data are not unique, i.e., a different data set is obtained with each different method used. As a consequence of the accumulated modifications of the original data, the original error characteristics are lost. The variance-covariance matrix of the new data set entering the least-squares adjustment must be then supplied in some approximate fashion.

A more rigorous approach would be to utilize the original observations together with their variance-covariance matrix. This can be done by differencing the range-rate observations at some suitable time intervals. In particular, one has

$$[\dot{R}(t+\Delta t) - \dot{R}(t)]/\Delta t = \ddot{R}(t) + o ,$$

$$o = (1/2)(d\ddot{R}/dt)\Delta t + \dots$$

In considering the previous outcome, the SST adjustment model becomes

$$[\dot{R}(t+\Delta t) - \dot{R}(t)]/\Delta t = (\nabla V_2 - \nabla V_1) \cdot \underline{e} + o + b . \quad (1)$$

This model relates a combination of observations (two per equation) to the parameters of the gravity field and to the small corrections o and b .

Transformation of the SST Adjustment Model

An adjustment model represented by a system of equations encompassing both the observables and the parameters is described in general by

$$f(X^a, L^a) = 0 , \quad (2)$$

where, according to the standard adjustment notation, $X^a = X^0 + X$ and $L^a = L^b + V$. The sets (column-vectors) X^a , X^0 , and X contain the values of adjusted parameters, initial parameters, and parametric corrections, respectively; and the sets L^a , L^b , and V represent adjusted observations, actual observations, and residuals, respectively. It is an ongoing practice that a model such as (2) is linearized upon neglecting higher-order terms in its Taylor series expansion. This gives rise to the matrix equation

$$A X + B V + W = 0 , \quad (3)$$

where $A = \partial f / \partial X$ and $B = \partial f / \partial L$, both evaluated with X^0 and L^b , and where $W = f(X^0, L^b)$. The matrices A and B are assumed to have the full column rank and the full row rank, respectively. Equation (3) characterizes the standard setup of the general adjustment method, which is resolved in accordance with the least-squares principle.

The neglect of higher-order terms in the Taylor series expansion of a nonlinear model represents the greatest simplification and, at the same time, the greatest shortcoming of the standard adjustment theory. The price to pay for such a simplification is represented either by non-rigorous results if the solution is not iterated, or by the necessity to iterate the least-squares

algorithm. Depending on how severe is the model's nonlinearity, the iterative process may be slow to converge. Thus, in theory, equation (3) should read

$$A X + B V + W + \dots = 0 , \quad (4)$$

where the dots represent the contribution of nonlinear terms due, in general, to the model's nonlinearity in both the observables and the parameters.

If, however, the observables (but not the parameters) are combined in a linear fashion, (2) can be written in a different functional form, namely

$$\bar{L}^a = B L^a = F(X^a) , \quad (5)$$

where the symbol \bar{L}^a represents "transformed adjusted observations". The new matrix B is again assumed to have the full row rank. Since $L^a = L^b + V$ and $\bar{L}^a = \bar{L}^b + \bar{V}$, where \bar{L}^b symbolizes "transformed observations" and \bar{V} symbolizes "transformed residuals", one has

$$\bar{L}^b = B L^b , \quad \bar{V} = B V . \quad (6a,b)$$

If the model (5) is now linearized in the parameters, it results in the following system of observation equations:

$$\bar{V} = A X + L , \quad (7)$$

where

$A = \partial F / \partial X$ = design matrix (evaluated with the initial set X^0),

$X = X^a - X^0$ = vector of parametric corrections, and

$L = F(X^0) - \bar{L}^b = F(X^0) - B L^b$ = vector of constant terms.

The variance-covariance matrix $\bar{\Sigma}$ of transformed observations \bar{L}^b is formed rigorously from (6a) as

$$\bar{\Sigma} = B \Sigma B^T , \quad (8)$$

where Σ is the variance-covariance matrix of the actual observations L^b . The adjustment of the linearized parametric model (7) would proceed with the proper variance-covariance matrix from (8), whose inverse would be the weight matrix of transformed observations and would be used in the formation of normal equations. The shortcoming associated with the linearization of a nonlinear adjustment

model has been discussed at the outset of this section. Thus, in theory, equation (7) should read

$$\bar{V} = A X + \dots + L, \quad (9)$$

where the dots represent the contribution of nonlinear terms due to the model's nonlinearity in the parameters.

The SST adjustment model presented in (1) has the form equivalent to (9). This stems from the fact that the observations represented by the left-hand side of (1) conform to the linear pattern (6a). In particular, the left-hand side of an i -th equation is formed as $(1/\Delta t) \times (\text{observation } i+1) - (1/\Delta t) \times (\text{observation } i)$. With a constant Δt , the matrix B would have the form

$$B = (1/\Delta t) \begin{bmatrix} -1 & 1 & 0 & 0 & \dots \\ 0 & 1 & 1 & 0 & \dots \\ \vdots & & & & \\ \vdots & & & & \end{bmatrix}.$$

With the aid of this matrix and of the rigorous variance-covariance matrix Σ of range-rate measurements, one forms the rigorous variance-covariance matrix $\bar{\Sigma}$ as indicated in (8), which is then to be used in the parametric least-squares adjustment of the SST model.

The SST model is in general nonlinear in the parameters, with the degree of nonlinearity depending on the type of parameters expressing the desired components of the earth's gravity field and other phenomena. This, together with the above outcome, has compelled the analysis to shift focus from the general adjustment model to the nonlinear parametric adjustment model. With the provision of using the proper variance-covariance matrix from (8), the overbars are dropped and the parametric model is written as

$$L^a = F(X^a) = F(X^0) + A X + \dots \quad (10)$$

This model is alternately presented in the form (9), which now reads

$$V = A X + \dots + L, \quad (11)$$

where

$$V = L^a - L^b = \text{vector of residuals,}$$

$$A = \partial F / \partial X = \text{design matrix (evaluated with the initial set } X^0),$$

$X = X^a - X^0$ = vector of parametric corrections, and

$L = F(X^0) - L^b$ = vector of constant terms.

The variance-covariance and the weight matrices of observations are denoted Σ and P , respectively, where $P = \Sigma^{-1}$. There exist an infinite number of sets L^a consistent with the model (10). Of these, the least-squares principle selects the one fulfilling $V^T P V = \text{minimum}$.

APPENDIX B

LINEAR PARAMETRIC ADJUSTMENT MODEL WITH LINEAR INEQUALITY CONSTRAINTS

Introduction to Adjustment with Inequality Constraints

When used in conjunction with a parametric adjustment model, inequality constraints limit the domain of selected parameters or functions thereof. Qualitatively, this property reminds one of the familiar equality constraints, where the individual signs $=$ would now be replaced by the signs \geq or \leq . However, a set of inequality constraints is in general less restrictive than its equality counterpart because only a subset of the former changes into a subset of the latter in the course of adjustment computations. The constraints having this property (i.e., whose signs \geq or \leq have changed into the sign $=$) are called binding; their number may range from zero to the total number of the original constraints. The remaining constraints are called nonbinding, and they have no effect on the adjustment.

The basic, and perhaps the most common, kind of inequality constraints consists of upper or lower bounds imposed on linear combinations of parameters, including the class of upper or lower bounds imposed on selected parameters themselves. An imposition of known lower bounds on selected parameters, for example, can be an important asset if this is dictated by physical or mathematical reality. One cannot include such vague information into the adjustment process by weighting the parameters in question, since this would necessitate their a priori estimates as well as the variance-covariance matrix associated with such estimates. On the other hand, discarding this or similar information might lead to results inconsistent with the reality. One can then decide to either forego the inclusion of inequality constraints in the hope that such an inconsistency will be small or nonexistent due to appropriate measuring and modeling techniques, or to incorporate these constraints into a rigorous least-squares adjustment and thereby transform the hope into certainty.

Adjustment using bounds on specific parameters or their combinations is increasingly finding its niche in geodesy, photogrammetry, oceanography, and in many other sciences. For example, one of the most recent photogrammetric

applications is concerned with digital object reconstruction. It has been noted that the standard (linear) least squares method is often insufficient because of its smoothing effect. A suitable alternative has been considered in terms of "Chebyshev formulation", which represents a generalization of this method. In recent reports and papers, such as [Fritsch, 1987], this formulation is achieved by using the concept of least-squares adjustment with inequality constraints, where both the parametric model and the constraints are linear. The purpose of such a development is to reduce the solution space to a band, which, in turn, allows one to minimize the maximum error, i.e., to accommodate the worst case. According to Fritsch [1987], the inequality-constrained least-squares adjustment was introduced into geodesy by B. Schaffrin in 1981.

As a plausible oceanographic illustration with bounds imposed on the parameters, we mention the action spectral density of fluctuations of sea surface elevation, which is a non-negative quantity over all spectral bands. The sea surface fluctuations have been studied by Snyder [1988], who utilizes the linear relation $A = \sum A_i G_i$, where A is the action spectral density, A_i are parameters (to be determined from observations), G_i are basis functions, and where the summation extends over the spectral bands considered, $i=1,2,\dots$. In a convenient approach, the spectral representation is adopted as piecewise continuous, such that $G_i=1$ inside the i -th spectral band and $G_i=0$ elsewhere. The key consideration pertinent to our discussion resides in the fact that should $A \geq 0$ hold true everywhere, all of the parameters A_i are required to be non-negative. Thus, the condition $A_i \geq 0$, $i=1,2,\dots$, represents a basic case of linear inequality constraints.

Motivated by the above considerations, the present study has focused on linear inequality constraints. Due to complexities associated with nonlinear least-squares adjustment, certain aspects of which are treated in [Blaha, 1989], the analysis has been further restricted to applications involving linear parametric adjustment. Upon taking advantage of a geometrical setup reflecting the situation where a linear model is to be resolved in conjunction with linear inequality constraints, a new, yet relatively simple algorithm has been derived producing a unique least-squares estimate. A similar isomorphic geometrical setup can undoubtedly serve in the future in resolving also nonlinear adjustment models in conjunction with linear and even nonlinear inequality constraints.

Matrix Formulation of Linear Inequality Constraints

In this section, we present some of the outcome of the study which will be described in the AFGL Scientific Report No. 2, *Linear Parametric Adjustment Model with Linear Equality and Inequality Constraints*. Although the algorithm for resolving the linear adjustment model with linear inequality constraints has been derived using geometry with tensor structure and notation, here the results are presented in the standard matrix notation. The inequality constraints have the form of lower bounds, since upper-bound constraints can be transformed into lower-bound constraints upon multiplying the pertinent inequality by -1.

The linear parametric adjustment model, before the introduction of any constraints, reads

$$L^a = L^b + V = A X + L^0 ,$$

where the column-vector L^a contains n adjusted observations, L^b contains n actual observations, V contains n residuals, L^0 contains n constant values, and the column-vector X contains u parameters, $u < n$. The symbol A denotes the design matrix of dimensions $n \times u$, assumed to have the full column rank u . The above relation is often written in the form of observation equations

$$V = A X + L , \quad (1)$$

where $L = L^0 - L^b$. When subjected to the least-squares criterion

$$V^T P V = \text{minimum} , \quad (2)$$

where P is the weight matrix of observations adopted as the inverse of Σ , the variance-covariance matrix of observations, (1) yields the normal equations

$$N X = U , \quad (3a)$$

with

$$N = A^T P A , \quad U = - A^T P L ; \quad (3b,c)$$

here N is a positive-definite matrix of dimensions $u \times u$ and U is a column-vector of u elements.

The scope of a study concerned with linear inequality constraints can be narrowed down in two ways. First, the constraints can be treated in the form

$$C X \geq 0 , \quad (4)$$

where C is a matrix of dimensions $s \times u$, with $s \leq u$, assumed to have the full row rank s . Since, in general, $X = X^a X^0$, where X^a symbolizes the adjusted parameters and X^0 symbolizes the initial values of parameters, the cases such as $CX \geq c$, where c is a constant vector of s elements, can be transformed into (4) upon properly modifying the values in X^0 .

The second simplification can be achieved through a unique linear parametric transformation carrying the vector X into a vector Y , likewise composed of u elements. In particular, upon partitioning X and Y into $u-s$ and s elements, and attributing the subsets a prime and a double prime, respectively, we have

$$Y' = X' ,$$

$$Y'' = C' X' + C'' X'' \geq 0 ,$$

where C has similarly been partitioned into the submatrices C' and C'' . The second equation above is equivalent to (4). From these relations one can express X' and X'' in terms of Y' and Y'' , and use the result in (1), yielding

$$V = A' Y + L ,$$

where A' follows from A and from the transformation coefficients. We note that C'' has been assumed to be a regular matrix (i.e., square and nonsingular). Due to the full row rank of C , this assumption is justified, either initially or upon renumbering the parameters. After the vector Y and its variance-covariance matrix Σ_Y have been determined, the parametric transformation yields the original vector X , and the law of variance-covariance propagation yields Σ_X .

In order to reduce the number of symbols, we change the notation from A' to A , and from Y to X . The last two equations are then transcribed as

$$V = A X + L , \tag{5a}$$

$$X'' \geq 0 , \tag{5b}$$

where X'' is a subset of X . If X'' comprises the full set X , the adjustment model with constraints becomes

$$V = A X + L , \tag{6a}$$

$$X \geq 0 . \tag{6b}$$

This is, in fact, the basic problem discussed in the previous section, where all the parameters were required to be non-negative. However, this case is quite suitable for a general treatment of linear inequality constraints, since disregarding the pertinent u-s constraints in (6b) leads to the system (5a,b), which, in turn, is equivalent to the system (1), (4).

Outline of the Geometrical Approach

The derivations summarized in this section will appear in the above-cited report. In the geometrical context, the n observations grouped in L^b correspond to the coordinates of the "observational point" Q lying in an n -dimensional flat "observational space". Since the metric tensors of all the manifolds considered here are constant (due to the linear setup), we can interpret coordinates of a point as contravariant components of its position vector, and coordinate lines as oblique Cartesian axes with constant individual scales. The matrices Σ and P (constant) correspond respectively to the associated metric tensor and to the metric tensor of the observational space. The u initial parametric values in X^0 correspond to the coordinates of the "initial point" P_0 . The latter lies in the known u -dimensional flat "model surface", also called "model hyperplane", which is embedded in the observational space. In an unrestricted least-squares (L.S) adjustment, the adjusted parameters X^a correspond to the point denoted P , which likewise lies in the model surface. The adjustment notation X then designates the contravariant components of the vector P_0P . Due to constant metric tensors of the observational space and of the model surface, vectors in these manifolds can be freely parallel-transported to any location. This allows us to identify P_0 throughout the analysis, with the coordinate origin in the model surface.

The unrestricted L.S. solution represented by the point P is obtained by projecting the observational point Q onto the known u -dimensional model hyperplane. Here the term "projection" will always be synonymous with "orthogonal projection". The L.S. solution subject to inequality constraints would be obtained by projecting Q onto another surface, as yet unknown, and generating the point denoted \bar{P} . Clearly, in the absence of constraints, or in the presence of only nonbinding constraints, P and \bar{P} would coincide. But since, in general, the constraints (5b) or (6b) limit the solution point to a region of the u -dimensional model hyperplane, the point P must be transferred in

some way into this "admissible" region. At the same time, in order to fulfill the L.S. criterion, the new point must coincide with \bar{P} .

The above discussion indicates that the point P , itself the result of a projection, must be further projected onto an "envelope" delimiting the admissible region. The transfer of P inside this region, or onto its envelope other than by a projection, would be inconsistent with the L.S. principle, which, in the geometrical context, translates into the shortest-distance principle. The form of (5b) or (6b) allows us to consider the "sides" of the above envelope as portions of lower dimensional hyperplanes embedded in the model hyperplane and spanned by combinations of coordinate axes. We will solve the inequality-constrained L.S. adjustment by projecting the unrestricted L.S. point P from the known u -dimensional model hyperplane onto a lower-dimensional "embedded hyperplane", thereby generating the point \bar{P} , in such a way that

- a) the latter hyperplane has the highest dimensionality possible;
- b) the line connecting P and \bar{P} does not pass through any part of the admissible region; and
- c) the point \bar{P} is consistent with the inequality constraints.

The thus generated constrained L.S. point \bar{P} is identical to the point which would be obtained via an orthogonal projection of the observational point Q directly onto the (unknown) lower dimensional hyperplane.

The determination of the unrestricted L.S. point P corresponds, in the adjustment context, to the solution of the normal equations (3a-c). If the parameters show conflict with the constraints represented by (5b) or (6b), P must be projected as discussed above. The geometrical algorithm developed for this purpose proceeds in accordance with the strategy summarized as follows:

- 1) Only the conflicting (negative) elements of X will induce projections. (Since it can be shown that any permutation of a given sequence of projections yields the same point, a sequence where only negative components have induced projections can be imagined in a different permutation, which now may include projections corresponding to positive components. This specific sequence would also yield the above point, but such arrangements are strictly avoided.)
- 2) The projections are "closely nested", in the sense that a point lying in a given hyperplane can only be projected onto a hyperplane whose dimensionality is

lower by one. This process is repeated until the constrained L.S. point \bar{P} is reached, or until a given sequence is rejected.

The point \bar{P} can be reached along different routes, or "branches", formed by allowable permutations in a successful sequence of projections. Similarly, one or more non-L.S. points (to be rejected) may be reached by many branches. It is thus important to avoid branches that are essentially repetitions. To this end, the geometrical algorithm will keep track, at each level, of the permutations that have already taken place. The level m is defined as the stage in the algorithm where the number of consecutive projections has reached m , and the dimensionality of the latest hyperplane is $u-m$. If, for example, a given branch includes the projections symbolized by the letters a, b, and c, another branch containing the projections c, a, b will be discarded at the third level. As another example, if the projection sequence g, h is rejected, the sequence h, p, q, g will be automatically rejected since it contains the forbidden combination g and h.

One of the crucial elements in the geometrical algorithm is the early detection of branches that should be rejected. The rejection criterion will be provided by a "guide vector" of u elements, which will contain the differences, in model-surface covariant components, between a projected point and the unconstrained L.S. point P . It can be shown that the elements in the guide vector must be ≥ 0 , otherwise the pertinent branch leads to a non-L.S. point. This property can be first demonstrated for the constrained L.S. point \bar{P} , which can be thought of as lying in a $u-m$ dimensional hyperplane. Since \bar{P} is the result of an appropriate orthogonal projection (composed of m "closely nested" projections) of P onto this hyperplane, a u -dimensional sphere centered at P and having the smallest possible radius touches the hyperplane at \bar{P} . At this stage, we introduce a $u-1$ dimensional hyperplane, called the \bar{P} -divider, which is tangent to this sphere at \bar{P} and generates two u -dimensional half spaces. The \bar{P} -divider itself contains the $u-m$ dimensional hyperplane of the point P .

If all the coordinate axes are parallel-transported from the origin to \bar{P} , $u-m$ of them will lie in the above $u-m$ dimensional hyperplane (always containing the axes of coordinates not subject to constraints), and the remaining m must lie in the half-space excluding the point P . But this means that the cosine of the angles formed by the vector $P\bar{P}$ and by any of the u coordinate axes must be

either 0 (with regard to the $u-m$ axes spanning the $u-m$ dimensional hyperplane of \bar{P}), or larger than zero (with regard to the remaining m axes). This, in turn, leads to $u-m$ zeros and to m values larger than zero in the corresponding entries of the guide vector formed for the constrained L.S. point \bar{P} .

The intermediate points formed by the projections that ultimately generate \bar{P} can be thought of as a sequence of nested L.S. problems with certain constraints removed. Therefore, the entries of the guide vectors associated with the intermediate points along a given branch must be ≥ 0 , otherwise this branch will not result in the L.S. point \bar{P} and should be rejected. Since a (u -dimensional) sphere touches a hyperplane of any dimensions in one point only, there can be only one L.S. point \bar{P} . In conclusion, if any branch reaches a point for which all components subject to constraints are ≥ 0 , and for which all guide-vector entries are ≥ 0 , this point is \bar{P} . The unique L.S. solution has thus been found and all the remaining branches should be discontinued.

Description of the Geometrical Algorithm

The unrestricted L.S. solution X (i.e., a column-vector of u elements corresponding to the point P) is computed from (3a) as

$$X = N^{-1} U. \quad (7)$$

It would have been formally more appropriate to denote the unrestricted L.S. solution by a different symbol, e.g. $X^{(0)}$, and to reserve the symbol X for the constrained L.S. solution. However, the geometrical algorithm will be described more conveniently with the unrestricted solution represented by X , and with the constrained solution attributed superscripts in parentheses. We now partition X into $u-1$ elements and into the remaining one element, for example the last, and partition the column-vector U in the same way. Similarly, the matrix N is partitioned into the leading submatrix of dimensions $(u-1) \times (u-1)$ and into the remaining submatrices of dimensions, clockwise, $(u-1) \times 1$, 1×1 (a single number), and $1 \times (u-1)$. These partitions are symbolized by

$$X = \begin{bmatrix} X_1 \\ X_u \end{bmatrix}, \quad U = \begin{bmatrix} U_1 \\ U_u \end{bmatrix}, \quad N = \begin{bmatrix} N_{11} & N_{1u} \\ N_{u1} & N_{uu} \end{bmatrix}, \quad (8a,b,c)$$

where X_u , U_u , and N_{uu} are single numbers.

It should be borne in mind that the subscript "1" does not correspond to one element, or to the first element, but to a set of $u-1$ elements, here the first $u-1$ of u elements. On the other hand, the subscript "u" pertains to one element, here the last of u elements. Since the matrix N is positive-definite, so are its diagonal submatrices N_{11} and N_{uu} ; here, in particular, $N_{uu} > 0$. The submatrices N_{u1} and N_{1u} are transposes of each other. A computational advantage stemming from an arrangement such as (8c) is that

$$N_{uu}^{-1} = 1/N_{uu} \quad (8d)$$

the reciprocal value of a number. Most importantly, partitions of this kind correspond to the geometrical strategy of closely nested projections. The formulas presented in matrix notation in the remainder of this section have been developed via geometry, although some of them can be derived, in a more tedious manner, also by algebraic means.

If the unrestricted L.S. solution produces $X_u < 0$, the constraint $X_u = 0$ may be binding. Henceforth we assume the constraints (6b), or (5b) where X_u belongs to the set X . Thus, a reference to an element as being "negative" implies "conflicting negative". Should the above constraint be indeed binding, it would induce a projection onto the appropriate hyperplane of dimensions $u-1$. This possibility should be scrutinized in an appropriate branch. As an example, in a three-dimensional model hyperplane with oblique Cartesian axes $\{x, y, z\}$, an unconstrained result $z < 0$ (with respect to P_0 as the origin) would induce the projection of P onto the plane $\{x, y\}$ in one of possible branches.

In considering X_u as the last parameter, the projection of P onto the hyperplane spanned by the first $u-1$ coordinate axes can be shown to be equivalent to solving

$$X_1^{(1)} = N_{11}^{-1} U_1, \quad X_u^{(1)} = 0 \quad (9a, b)$$

where, in analogy to (8a), $X_1^{(1)}$ contains $u-1$ elements and $X_u^{(1)}$ is a single number. The variance-covariance matrices for these two subsets are N_{11}^{-1} and 0, respectively. However, instead of inverting N_{11} at the first level, and inverting progressively smaller matrices at further levels, one can take advantage of the property paralleling (8d) and deduce

$$N_{11}^{-1} = N^{11} - N^{1u} (1/N^{uu}) N^{u1} \quad (10)$$

where N^{11} , N^{1u} , N^{uu} , and N^{u1} are submatrices of N^{-1} ; the latter is imagined to be partitioned in a complete analogy to (8c), except that the superscripts now replace the subscripts.

We next attribute to X a superscript in parentheses, indicating the level of the algorithm, i.e., the number of projections effectuated up to and including the current step. This notation has already been used in (9a,b) above for the first level of projections. In general, the notation $X_1^{(m)}$ identifies a vector of $u-m$ elements obtained at the m -th level; the remaining m elements in the complete vector $X^{(m)}$ are zero. The elements brought to zero by successive projections are not, in general, the last elements in given partitions as was assumed in (8a-d) and (9a,b) for convenience. Instead, they are the negative elements which have effectively induced such projections. However, their location in X or its subsequent partitions does not alter the architecture of formulas such as (10). We only have to make sure that N^{uu} corresponds to the negative element inducing the (next) projection. It is now denoted N^{ii} , where the generic index "i" symbolizes the negative element in question. Clearly, N^{ii} may correspond to the last element as well, provided the latter turns out to be negative, and provided we are treating the branch where this element actually induces a projection. This reflects the possibility that there may exist other negative elements in X , each of which may induce a legitimate (non-repetitious) projection and thereby create a separate branch.

The submatrices of the type N_{11}^{-1} will also be attributed a superscript in parentheses, likewise indicating the level of projections. Thus, N_{11}^{-1} is written as $N^{(1)}$, to be potentially partitioned into the submatrices denoted $N^{(1)11}$, $N^{(1)1i}$, $N^{(1)ii}$, and $N^{(1)i1}$, and equation (10) is rewritten as

$$N^{(1)} = N^{11} - N^{1i} (1/N^{ii}) N^{i1} \quad (11)$$

The lack of superscripts in parentheses on the right-hand side of (11) is equivalent to a superscript "(0)". This means that no modification has taken place as yet, and, accordingly, that N^{11} , N^{1i} , N^{ii} , and N^{i1} are submatrices of the original matrix N^{-1} . In general, we have

$$N^{(m)} = N^{(m-1)11} - N^{(m-1)1i} [1/N^{(m-1)ii}] N^{(m-1)i1} \quad (12)$$

where the dimensions of $N^{(m)}$ are $(u-m) \times (u-m)$. The dimensions of $N^{(m-1)11}$ are the same, while the dimensions of $N^{(m-1)1i}$ and $N^{(m-1)i1}$ are respectively $(u-m) \times 1$ and $1 \times (u-m)$. Predictably, $N^{(m-1)ii}$ is a single number regardless of m .

Although the vector U has served in obtaining the unrestricted L.S. solution in (7), it will not be used in any capacity for any other task. This stems from the fact that the geometrical algorithm avoids new matrix inversions, such as featured in (9a), and takes advantage instead of the relations such as (12), involving relatively very few scalar multiplications. In lieu of (9a), the first-level solution is given by the algorithm as

$$X_1^{(1)} = X_1 - N^{1j} (1/N^{11}) X_j, \quad (13)$$

and in lieu of inverting N_{11} , one can obtain the variance-covariance matrix associated with this solution as in (11). In general, the m -th level solution is given by the algorithm as

$$X_1^{(m)} = X_1^{(m-1)} - N^{(m-1)1i} [1/N^{(m-1)ii}] X_i^{(m-1)}, \quad (14)$$

with the corresponding variance-covariance matrix $N^{(m)}$ presented in (12). The remaining m elements in $X^{(m)}$ are zero, and the pertinent variance-covariance matrix is a zero matrix.

We notice that not only does the path from (11) to (12) involve relatively few scalar multiplications as has already been mentioned, but these operations take place in successively smaller systems. A similar statement applies also when proceeding from $X_1^{(1)}$ to $X_1^{(m)}$. We reiterate that the generic index "i" in all of the above formulas identifies a negative element of the solution vector at a given level. This element is necessarily different from level to level. In fact, once a negative element has been suppressed by a projection, it becomes zero and remains fixed at that value.

Without the aid of the guide vector, we would attempt to reach the constrained L.S. solution subject to (6b), for example, by examining various branches while avoiding equivalent (i.e., essentially repetitious) paths. This would lead to one or more solutions at a given level, e.g. the level m , the elements of which would be all non-negative. The values of $\Delta V^T PV$ due to each projection along an individual path would be accumulated and added to the value of $V^T PV$ from (2), associated with the unrestricted adjustment. The decisions as to whether a given outcome is a L.S. solution, and as to which branches can be

discontinued at what level, would then be made based on the accumulated $V^T PV$. The increment in $V^T PV$ due to the m -th projection is very simple to compute (it is, in fact, already partially evaluated in equation 14):

$$\Delta V^T PV^{(m)} = [1/N^{(m-1)}]_{ij} [X_i^{(m-1)}]^2 \quad (15a)$$

Based on (15a), the accumulated $V^T PV$ is computed as

$$V^T PV^{(m)} = V^T PV + \Delta V^T PV^{(1)} + \Delta V^T PV^{(2)} + \dots + \Delta V^T PV^{(m)} \quad (15b)$$

If a certain branch yielded $X^{(m)} \geq 0$, all the branches where the accumulated value of $V^T PV$ has surpassed the current value (15b) for this solution would be discarded. The remaining branches would be continued, since the accumulated $V^T PV$ in one or more of them could be smaller than the current value (even though they might entail more than m projections). If the latter should occur, it would indicate, in turn, that the current branch has resulted in a non-L.S. solution. In spite of the simplicity of (15a,b), this strategy has the drawback that it discards a branch "after the fact", i.e., after an additional projection has been computed.

In this context, the guide vector acts as an invisible arm reaching forward into the next projection and detecting a possible cause for rejection (when one or more of the vector's elements are negative). Suppose that the current m -th level has resulted in the solution $X_1^{(m)}$, obtained upon using $N^{(m-1)}$, etc., according to (14). Suppose further that some of the elements in $X_1^{(m)}$ are negative. However, instead of a complete formulation of one distinct matrix $N^{(m)}$ associated with each negative element in view of computing distinct vectors $X_1^{(m+1)}$ and giving rise to distinct branches, we compute only one diagonal element of each such matrix $N^{(m)}$.

For the sake of illustration, we consider one (possibly the only) negative element of $X_1^{(m)}$, which we symbolize by "j", i.e., we consider the element $X_j^{(m)} < 0$. (The negative element at the previous level was $X_i^{(m-1)}$.) The current negative element $X_j^{(m)}$ has the potential to generate the branch "j" at the next level, numbered $m+1$. This branch, if treated, will require the knowledge of the pertinent matrix $N^{(m)}$ in order to compute the solution vector $X_1^{(m+1)}$. However, we only compute the j -th diagonal element of $N^{(m)}$, which is needed as a building block of the guide vector at this stage. In denoting it $N^{(m)}_{jj}$ and consulting (12), we deduce that

$$N^{(m)}_{jj} - N^{(m-1)}_{jj} - [N^{(m-1)}_{ji}]^2 [1/N^{(m-1)}_{ii}] . \quad (16)$$

The remaining elements of $N^{(m)}$ for the branch "j" will be computed only if this branch is not rejected by the guide vector.

We are now in a position to complete the formation of the guide vector. As has been explained, this vector's role is to examine, from a given level, a potential projection to be performed at the next level. The guide vector is the most easily formed at the level 1, although at this level it cannot provide any service as will become clear presently. In assuming that the element "i" in the original vector X is negative, $X_i < 0$, and in proceeding along this branch, one can show that all the entries of the guide vector at the first level are zero except for the entry "i", which is positive. The latter is obtained as

$$G_i^{(1)} = (1/N^{11})(-X_i) > 0 . \quad (17)$$

Since $G^{(1)} \geq 0$ by construction, it is incapable of rejecting its branch.

We confirm the above assertion for a three dimensional model hyperplane with oblique Cartesian axes $\{x, y, z\}$, where an unrestricted L.S. point P has $z < 0$. The projection of P onto the plane $\{x, y\}$ generates the point P' , for which the first two covariant components of the guide vector are zero. Regardless of whether P' falls inside the desired (sub-)region $x \geq 0, y \geq 0$, the corresponding P' -divider is identical with the plane $\{x, y\}$, while the z -axis points away from the half-space of P ; the latter point is "below" the plane $\{x, y\}$ by virtue of $z < 0$. But since the z -axis and the guide vector are pointing into the same half-space, the third covariant component of this vector is positive. Similarly, P having a negative i -th coordinate may be projected from a u -dimensional model hyperplane onto a $u-1$ dimensional embedded hyperplane, generating P' as well as the corresponding P' -divider. The latter coincides with the embedded hyperplane and thus contains $u-1$ of the u coordinate axes, while the remaining axis "i" points away from the half space of P .

We next suppose that the element "j" of $X^{(1)}$ is negative, i.e., $X_j^{(1)} < 0$. Before proceeding to the full-scale computation at the second level (branch "j") necessitating $N^{(1)}$ in order to produce $X^{(2)}$, we compute the guide vector $G^{(2)}$ for such a solution in order to determine whether this branch should not be discarded altogether. The vector $G^{(2)}$ will have two entries different from zero

("i" and "j"), while all its remaining entries will be zero. The entry "j" will be positive, computed in analogy to (17):

$$G_j^{(2)} = [1/N^{(1)jj}] [-X_j^{(1)}] > 0, \quad (18)$$

where $N^{(1)jj}$ would be obtained from the formula (16) with $m=1$. The entry "i" is composed of two parts, namely the previous entry "i" plus a simple correction:

$$G_i^{(2)} = G_i^{(1)} - (1/N^{1i}) N^{ij} G_j^{(2)}. \quad (19)$$

If $G_j^{(2)}$ turns out to be negative (due to the correction), the branch "i", "j" is rejected. Otherwise one proceeds to complete $N^{(1)}$, leading to $X^{(2)}$.

If, in this case, an element "k" of the solution $X^{(2)}$ is negative, i.e., if $X_k^{(2)} < 0$, we generate the guide vector $G^{(3)}$ to test the third level. This vector will have three nonzero entries, "i", "j", and "k". The entry "k" is positive, computed in analogy to (17) or (18):

$$G_k^{(3)} = [1/N^{(2)kk}] [-X_k^{(2)}] > 0, \quad (20)$$

where $N^{(2)kk}$ would be readily obtained from (16) with $m=2$ and with j and k replacing i and j, respectively. The entry "j" is composed of the previous entry "j" plus a simple correction (one term):

$$G_j^{(3)} = G_j^{(2)} - [1/N^{(1)jj}] N^{(1)jk} G_k^{(3)}. \quad (21)$$

Clearly, the elements $N^{(1)jj}$, $N^{(1)jk}$, etc., are available from the previous level (see the statements following equation 19). Finally, the entry "i" is composed of the previous entry "i" plus a correction consisting of two terms:

$$G_i^{(3)} = G_i^{(2)} - (1/N^{1i}) [N^{ij} G_j^{(3)} + N^{ik} G_k^{(3)}]. \quad (22)$$

It is noteworthy that all the building blocks needed in (20)-(22) are available, whether beforehand or sequentially, with the exception of $N^{(2)kk}$, which requires a very simple computation as indicated above.

The hierarchy in building the guide vector at higher levels is now quite apparent. The most recent entry in $G^{(m)}$ is always positive, and its computation requires an element obtainable via (16). The next most recent (nonzero) entry in $G^{(m)}$ is the corresponding entry in $G^{(m-1)}$ plus one correction term. The following entry in $G^{(m)}$ is the corresponding entry in $G^{(m-1)}$ plus two correction terms, etc. The correction terms in the last nonzero entry of $G^{(m)}$ contain

elements of the original matrix N^{-1} , i.e., elements belonging to the level "0". If any entry in $G^{(\ell)}$ is negative at any level, $\ell=2,3,\dots,m,\dots$, the pertinent branch is rejected. We recall that if any branch contains a permutation of a sequence of projections already rejected, such a branch should be discarded without testing.

Numerical Example Solved by the Geometrical Algorithm

The simple example below is presented at the level of normal equations (3a), where the inequality constraints have the form (6b):

$$N X = U, \quad (23a)$$

$$X \geq 0. \quad (23b)$$

The number of parameters is four, i.e., $n=4$. The matrix N and the vector U are given as

$$N = \begin{bmatrix} 1 & 0.5 & 0 & -3.75 \\ 0.5 & 1 & 1 & 0 \\ 0 & 1 & 4 & 4 \\ -3.75 & 0 & 4 & 25 \end{bmatrix}, \quad U = \begin{bmatrix} 0.675 \\ 0.35 \\ 0.2 \\ -5.1 \end{bmatrix}. \quad (24a,b)$$

The matrix N is positive-definite, and as such can be decomposed into the product $T^T T$, where the (real) matrix T is regular, upper-triangular.

The unrestricted L.S. solution, denoted X in agreement with an earlier convention, follows from (23a):

$$X = N^{-1} U. \quad (25)$$

In particular, we have

$$N^{-1} = (1/173) \begin{bmatrix} 944 & -432 & -40 & 148 \\ -432 & 444 & -55 & -56 \\ -40 & -55 & 75 & -18 \\ 148 & -56 & -18 & 32 \end{bmatrix}, \quad X = \begin{bmatrix} -1.6 \\ 0.8 \\ 0.35 \\ -0.5 \end{bmatrix}. \quad (26a,b)$$

The positive-definite matrix N^{-1} can be obtained from N as $T^{-1} (T^{-1})^T$, where T was introduced above; T^{-1} (real) is likewise regular and upper-triangular.

In applying the geometrical algorithm of the previous section, we replace the compact notation $X_1^{(1)}$ by a more explicit notation $[X^{(1)k}, X^{(1)\ell}, X^{(1)m}]^T$ when we need to identify specific elements. Thus, in the branch 1 below, $k=2$, $\ell=3$, and $m=4$. This kind of superscript notation will be used at any level (including the level 0), but only in conjunction with various vectors "X" and their subsets. Since $X^1 = -1.6$ and $X^4 = -0.5$, the level 1 will give rise to two branches, namely branch 1 (named after the element X^1) and branch 4 (named after the element X^4). Branch 1 will correspond to the possibly binding constraint $X^1 = 0$, or, more precisely, $X^{(1)1} = 0$, and to the projection of the unrestricted L.S. point P onto the three-dimensional hyperplane spanned by the second, third, and fourth coordinate axes. As has been just described, the vector $X_1^{(1)}$ is $[X^{(1)2}, X^{(1)3}, X^{(1)4}]^T$, while the corresponding vector X_1 is $[X^2, X^3, X^4]^T = [0.8, 0.35, -0.5]^T$. The solution $X_1^{(1)}$ then follows from (13), where $i=1$, i.e., where X_i is $X^1 = -1.6$. Similar comments with self-evident modifications apply also for the branch 4, where $i=4$.

If the branch 1 resulted in $X_1^{(1)} > 0$, and thus $X^{(1)} \geq 0$ (due to $X^{(1)1} = 0$), the unique constrained L.S. solution would be achieved. In this case, the guide vector $G^{(1)}$ composed of $G_1^{(1)}$ from (17) and of $n-1$ zeros would be unnecessary (all its entries would be ≥ 0). However, (17) would be a stepping stone in the computation of $\Delta V^T P V$ as given by (15a), since

$$\Delta V^T P V^{(1)} = G_i^{(1)} (-X_i), \quad (27)$$

where X_i is $X^1 = -1.6$ as above, with similar relationships occurring at higher levels as well. On the other hand, if the branch 1 does not lead to such a quick solution, guide vectors for the next level should be formed for all possible new branches.

Branch 1. In accordance with the above description, we form

$$\begin{bmatrix} X^{(1)2} \\ X^{(1)3} \\ X^{(1)4} \end{bmatrix} = \begin{bmatrix} 0.8 \\ 0.35 \\ -0.5 \end{bmatrix} - (1/173) \begin{bmatrix} -432 \\ -40 \\ 148 \end{bmatrix} (173/944)(-1.6) = \begin{bmatrix} 0.067797 \\ 0.282203 \\ -0.249153 \end{bmatrix}.$$

From $X^{(1)4} < 0$, we conclude that at least one more level will be needed. The next level (i.e., the level 2) will give rise to the branch 1,4. However, before proceeding any further, we form the guide vectors $G^{(1)}$ and $G^{(2)}$, the latter to

test whether the branch 1,4, and thus the entire branch 1, should not be rejected. First, (17) yields

$$G_1^{(1)} = (173/944) \times 1.6 = 0.293220 ,$$

from which it follows that $\Delta V^T PV^{(1)} = 0.469153$. In view of $G^{(2)}$, we compute $N^{(1)44}$ via (16) with $m=1$, upon the substitution $i=1$ and $j=4$:

$$N^{(1)44} = (1/173)(32 - 148^2/944) = 0.050847 .$$

With this entry, (18) and (19) yield

$$G_4^{(2)} = (1/0.050847) \times 0.249153 = 4.9 ,$$

$$G_1^{(2)} = 0.293220 - (173/944)(148/173) \times 4.9 = -0.475 .$$

Accordingly, the entire branch 1 is rejected.

Branch 4. This branch corresponds to the possibly binding constraint $X^{(1)4} = 0$. In analogy to the preceding procedure, we have

$$\begin{bmatrix} X^{(1)1} \\ X^{(1)2} \\ X^{(1)3} \end{bmatrix} = \begin{bmatrix} -1.6 \\ 0.8 \\ 0.35 \end{bmatrix} - (1/173) \begin{bmatrix} 148 \\ -56 \\ -18 \end{bmatrix} (173/32)(-0.5) = \begin{bmatrix} 0.7125 \\ -0.075 \\ 0.06875 \end{bmatrix} .$$

The only possible branch at the level 2 is 4,2. We notice that since the branch 1,4 was rejected above, so would be the branch 4,1; but the latter would now correspond to "projecting a positive component", which had been eliminated from the strategy. In view of the guide vectors $G^{(1)}$ and $G^{(2)}$, we compute

$$G_4^{(1)} = (173/32) \times 0.5 = 2.703125 ,$$

from which it follows immediately that $\Delta V^T PV^{(1)} = 1.351562$. Further, with $m=1$ and the substitution $i=4$ and $j=2$, equation (16) yields

$$N^{(1)22} = (1/173)(444 - 56^2/32) = 2 .$$

With this element, it follows from (18) and (19) that

$$G_2^{(2)} = (1/2) \times 0.075 = 0.0375 ,$$

$$G_4^{(2)} = 2.703125 - (173/32)(-56/173) \times 0.0375 = 2.76875 .$$

Thus, the branch 4,2 at the level 2 will not be rejected. Furthermore, upon considering (15a), the above result for $G_2^{(2)}$ yields $\Delta V^T PV^{(2)} = 0.002813$.

Branch 4,2. This branch corresponds to the possibly binding constraint $x^{(2)2} = 0$. We first use (11) with $i=4$ to compute $N^{(1)}$, which will serve to evaluate $x^{(2)}$:

$$N^{(1)} = (1/173) \left\{ \begin{bmatrix} 944 & -432 & -40 \\ -432 & 444 & -55 \\ -40 & -55 & 75 \end{bmatrix} - \begin{bmatrix} 148 \\ -56 \\ -18 \end{bmatrix} (1/32) [148 \quad -56 \quad -18] \right\},$$

$$N^{(1)} = \begin{bmatrix} 1.5 & -1 & 0.25 \\ -1 & 2 & -0.5 \\ 0.25 & -0.5 & 0.375 \end{bmatrix}.$$

This result is the same as the inverse of the (3×3) leading submatrix of N in (24a). However, the above scheme is much more economical, amounting to only a few scalar multiplications (advantage should be taken of the symmetry of N^{-1} , $N^{(1)}$, etc.).

With $N^{(1)}$ available, the solution $x_1^{(2)}$ follows from (14) as

$$\begin{bmatrix} x^{(2)1} \\ x^{(2)3} \end{bmatrix} = \begin{bmatrix} 0.7125 \\ 0.06875 \end{bmatrix} - \begin{bmatrix} -1 \\ -0.5 \end{bmatrix} (1/2)(-0.075) = \begin{bmatrix} 0.675 \\ 0.05 \end{bmatrix}.$$

Since these values are positive, the constrained L.S. solution has been achieved, namely

$$x^{(2)} = [0.675 \quad 0 \quad 0.05 \quad 0]^T.$$

According to (15b), the accumulated $V^T PV$ is

$$V^T PV^{(2)} = V^T PV + 1.351562 + 0.002813 = V^T PV + 1.354375.$$

We note that if the algorithm started with the branch 4, branch 4,2 would yield the unique constrained L.S. solution and branch 1 would be skipped altogether.

Description of the Quadratic Programming Algorithm

The L.S. adjustment of a linear parametric model with linear inequality constraints can be treated by the method of quadratic programming presented in [Bard, 1974], Section 6-2. In principle, the problem formulated on page 147 therein seeks to minimize the quadratic function Q in the parameters X , namely

$$Q(X) = X^T N X - 2 X^T U + c, \quad (28a)$$

subject to the inequality constraints

$$C X \geq 0. \quad (28b)$$

The dimensions of N , C , X , and U are respectively uxu , $s \times u$, $ux1$, and $ux1$. This task is equivalent to minimizing $V^T P V$ as in (2), subject to the constraints (28b). Accordingly, in terms of our notation, c in (28a) corresponds to $L^T P L$. It should be mentioned that the notation in [Bard, 1974] differs from that employed herein in several respects. For example, v corresponds here to X , R^{-1} corresponds to N , q corresponds to $-U$, etc.

As in (25), we denote the unrestricted L.S. solution by X and write

$$X = N^{-1} U.$$

The algorithm presented by Bard [1974] is transcribed below in our notation.

- 1) Form the matrix E of dimensions $s \times (s+1)$:

$$E \equiv [W \ z] = [C N^{-1} C^T \ C X]; \quad (29)$$

W is a matrix of dimensions $s \times s$, and z is a column-vector of s elements.

- 2) In conjunction with E , form the vector k of s elements, whose entries are initially set to unity.
- 3) Find the " i " for which $z_i k_i = a = \text{minimum}$; initially, a will be the smallest element of z . If $a \geq 0$, go to step 5.
- 4) If $a < 0$, execute the Gauss Jordan pivot on the element (i, i) of E , and change the sign of k_i . With the notation $t = 1/E_{ii}$, this pivoting consists of two basic steps, where " \rightarrow " symbolizes the replacement of elements:
 - a) For all the elements of E except the i -th row and the i -th column:

$$E_{pq} \rightarrow E_{pq} - E_{pi} E_{iq} t.$$

b) For all the remaining elements, starting with the i -th row except the element (i,i) :

$$E_{iq} \rightarrow E_{iq} t ;$$

continuing with the i th column except the element (i,i) :

$$E_{pi} \rightarrow -E_{pi} t ;$$

and ending with the element (i,i) :

$$E_{ii} \rightarrow t .$$

In fact, the three parts of the current item "b" could be performed in any order.

The new matrix E and the new vector k replace their previous counterparts, and, accordingly, are denoted again E and k . Within E , the symbols W and z are preserved as well. After the above replacements, return to step 3.

- 5) Suppose s' of the s elements in k are -1 (the others being $+1$). Form the matrix C' of dimensions $s' \times u$ from C , upon grouping the rows of the latter corresponding to the elements -1 in k . This procedure eliminates the rows of C corresponding to $+1$ in k , which represent nonbinding constraints. In the same way, form the column-vector z' of s' elements from z (z is the last column in the most recent matrix E). The constrained L.S. solution, denoted X' , is given as

$$X' = N^{-1} (U - C'^T z') . \quad (30)$$

Numerical Example Solved by the Quadratic-Programming Algorithm

The example used in this illustration is the one solved previously by the geometrical algorithm. Accordingly, $C=I$, $s=u=4$, and, from (29),

$$E = [W \ z] = [N^{-1} \ X] .$$

The values of N^{-1} and X are given in (26a,b). Thus, the initial matrix E and the initial vector k are

$$E = \begin{bmatrix} 5.456647 & -2.497110 & 0.231214 & 0.855491 & 1.6 \\ -2.497110 & 2.566474 & -0.317919 & -0.323699 & 0.8 \\ -0.231214 & -0.317919 & 0.433526 & -0.104046 & 0.35 \\ 0.855491 & -0.323699 & 0.104046 & 0.184971 & -0.5 \end{bmatrix}, \quad k = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}.$$

From this setup, the constrained L.S. solution will be reached in four iterations, in the sense that the computations will pass four times through step 3 of the quadratic-programming algorithm.

Iteration 1. The Gauss-Jordan pivot will be executed on the above element (1,1), for which $t = 1/5.456647 = 0.183263$. The matrix E and the vector k become

$$E = \begin{bmatrix} 0.183263 & -0.457627 & -0.042373 & 0.156780 & -0.293220 \\ 0.457627 & 1.423729 & -0.423729 & 0.067797 & 0.067797 \\ 0.042373 & -0.423729 & 0.423729 & -0.067797 & 0.282203 \\ -0.156780 & 0.067797 & -0.067797 & 0.050847 & -0.249153 \end{bmatrix}, \quad k = \begin{bmatrix} -1 \\ 1 \\ 1 \\ 1 \end{bmatrix}.$$

This iteration corresponds to the branch 1 of the geometrical solution.

Iteration 2. The pivoting will take place on the above element (4,4), for which $t = 1/0.050847 = 19.666667$.

$$E = \begin{bmatrix} 0.666667 & -0.666667 & 0.166667 & -3.083333 & 0.475 \\ 0.666667 & 1.333333 & -0.333333 & -1.333333 & 0.4 \\ -0.166667 & -0.333333 & 0.333333 & 1.333333 & -0.05 \\ -3.083333 & 1.333333 & -1.333333 & 19.666667 & -4.9 \end{bmatrix}, \quad k = \begin{bmatrix} -1 \\ 1 \\ 1 \\ -1 \end{bmatrix}.$$

This iteration would correspond to the branch 1.4 of the geometrical solution, if this branch had been executed. We note that the geometrical algorithm would have treated a smaller system at this stage, namely a 3×3 system. By contrast, the quadratic-programming algorithm treats essentially a 4×4 system at every iteration. We have seen that the guide vector allows the geometrical algorithm to avoid the (wasteful) execution of the branch 1.4, and directs it instead to the remaining branch 4.

Iteration 3. The pivoting will take place on the above element (1,1), for which $t = 1/0.666667 = 1.5$. This is the second time the element (1,1) is subject to the Gauss-Jordan pivot.

$$E = \begin{bmatrix} 1.5 & -1 & 0.25 & -4.625 & | & 0.7125 \\ 1 & 2 & -0.5 & 1.75 & | & 0.075 \\ 0.25 & -0.5 & 0.375 & 0.5625 & | & 0.06875 \\ 4.625 & -1.75 & 0.5625 & 5.40625 & | & -2.703125 \end{bmatrix}, \quad k = \begin{bmatrix} 1 \\ 1 \\ 1 \\ -1 \end{bmatrix}.$$

This iteration corresponds to the branch 4 of the geometrical solution.

Iteration 4. The pivoting in this last iteration will take place on the above element (2,2), for which $t = 0.5$.

$$E = \begin{bmatrix} 1 & 0.5 & 0 & 3.75 & | & 0.675 \\ -0.5 & 0.5 & -0.25 & 0.875 & | & -0.0375 \\ 0 & 0.25 & 0.25 & 1 & | & 0.05 \\ 3.75 & 0.875 & -1 & 6.9375 & | & -2.76875 \end{bmatrix}, \quad k = \begin{bmatrix} 1 \\ -1 \\ 1 \\ -1 \end{bmatrix}.$$

This iteration corresponds to the branch 4.2 of the geometrical solution, which yielded the constrained L.S. solution. From the above E and k, the quadratic-programming algorithm stipulates that

$$C' = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad z' = \begin{bmatrix} -0.0375 \\ 2.76875 \end{bmatrix}.$$

In using U from (24b), we obtain

$$U = C'^T z' = [0.675 \quad 0.3875 \quad 0.2 \quad 2.33125]^T.$$

Finally, (30) yields

$$X' = N^{-1} (U - C'^T z') = [0.675 \quad 0 \quad 0.05 \quad 0]^T,$$

whose first and third elements have already appeared at their respective places in the last column of E above. This solution X' agrees with the final result $X^{(2)}$ obtained in the branch 4.2 of the geometrical solution.

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